OPTIMAL ABSORBING BOUNDARY CONDITIONS
FOR FINITE DIFFERENCE MODELING OF
ACOUSTIC AND ELASTIC WAVE PROPAGATION

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ABSTRACT

An optimal absorbing boundary condition is designed to model acoustic and elastic wave propagation in 2D and 3D media using the finite difference method. In our method, extrapolation on the artificial boundaries of a finite difference domain is expressed as a linear combination of wave fields at previous time steps and/or interior grids. The acoustic and elastic reflection coefficients from the artificial boundaries are derived. They are found to be identical with the transfer functions of two cascaded systems: one is the inverse of a causal system and the other is an anticausal system. This method makes use of the zeros and poles of reflection coefficients in a complex plane. The optimal absorbing boundary condition designed in this paper yields about 10 dB smaller in magnitude of reflection coefficients than Higdon's absorbing boundary condition, and around 20 dB smaller than Reynolds' absorbing boundary condition. This conclusion is supported by a simulation of elastic wave propagation in a 3D medium on an nCUBE parallel computer.

INTRODUCTION

Absorbing boundary conditions are widely used in the numerical modeling of wave propagation in unbounded media to reduce reflections from artificial boundaries. Cerjan et al. (1985) and Reshef et al. (1988) used a method that enlarges a computational domain and applies damping mechanisms on the boundaries. Clayton and Engquist (1977) and Engquist and Majda (1979) developed a class of absorbing boundary conditions using the paraxial approximation to the wave equation, which are used frequently in the literature (Emerman and Stephen, 1983; Trefethen and Halpern, 1986; Levander, 1988; Renaut and Peterson, 1989; Dougherty and Stephen, 1991). Randall (1988, 1989) developed a boundary condition that converts displacements on the boundary to scalar
potentials and applies the absorbing condition of Lindman (1975) to individual potentials. Reynolds (1978) developed a class of absorbing boundary conditions by formal factorization of the differential operator for the acoustic wave equation. Good performances were reported in both acoustic and elastic forward modeling (Reynolds, 1978; Yoon and McMechan, 1992). Liao et al. (1984) developed a boundary extrapolation scheme that is closely related to Higdon’s space-time extrapolation method (Higdon, 1986). Both techniques dealt directly with difference equations other than differential boundary conditions that had to be discretized in their implementations. By cascading a series of first-order differential operators, Higdon (1987, 1990, 1991), Long and Liow (1990), and others proposed absorbing boundary conditions that give perfect absorption at certain angles of incidence, which are similar to those of Reynolds’ and are generalizations of those of Engquist and Majda (1979).

Stability is important in the choice of an absorbing boundary condition (Higdon, 1991). Emerman and Stephen (1983) showed that the second-order boundary condition of Clayton and Engquist (1977) was unstable for a wide range of elastic parameters. Mahrer (1986), in his empirical study of various types of absorbing boundary conditions, found the boundary conditions of Clayton and Engquist (1977) and Reynolds (1978), as well as certain type of Cerjan et al. (1985), to be unstable. Randall (1988) and Higdon (1991) reported that their boundary conditions are experimentally stable.

Besides stability, we are interested in a particular absorbing boundary condition that is optimal in the sense that maximum absorbing effect can be achieved with a minimum amount of computation and storage, and is easily implemented. This question is practical because, for instance, a 3D stress-velocity finite difference simulation of elastic wave propagation with an absorbing operator that involves m points deep in both time and space will require \( 9 \times 6 \times N \times N \times m \times m \times 4 \) bytes of memory. In this calculation, the 9 refers to the nine variables that need to be updated on the boundaries, the 6 refers to the six surfaces of a 3D volume, the 4 is the length in bytes of a real number on a computer, and \( N \) is the number of grids in each dimension. For a problem with \( 100 \times 100 \times 100 \) grids and \( m = 5 \), the memory for boundary grids is about 54 Mbytes. The total storage for interior grids, each is associated with 12 variables (3 particle velocities, 6 stresses and 3 elastic parameters), is 48 Mbytes in this example, even less than the amount of memory used on boundaries. The time spent on updating boundary grids is also significant compared to that spent on the interior grids.

In this paper, we will present an algorithm to design a class of optimal absorbing boundary conditions for a given operator length. As in Liao et al. (1984) and Higdon (1986), we employ directly a discrete formulation of extrapolation on a finite difference grid. Major motivation behind this decision is that the reflection coefficient of a discretized absorbing boundary condition differs from the corresponding continuous one by \( O(\omega \Delta t, \omega / \alpha \Delta x) \) (Higdon, 1986), which is not small for a typical computer simulation with \( \omega / \alpha \Delta x = 2\pi / 10 \sim 0.628 \) (i.e., 10 points per wavelength, where \( \omega \) denotes frequen-
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cy, α is the medium velocity, Δt the time step and Δx the grid size). We will show that for an absorbing boundary condition to be optimal, the zeros and poles of the reflection coefficients in a complex plane must lie on specific locations of the unit circle. A fast algorithm will be given to design useful absorbing boundary conditions.

THEORY

Problem Statement

Let \( v^n(k, j, i) \) denote a wavefield at \((z = kΔz, y = jΔy, x = iΔx)\) and at time \( t = nΔt \). In the interior of a finite difference domain, \( v \) is updated according to the difference approximations of wave equations. On the artificial boundaries, extrapolation based on values at previous time steps and/or interior grids is needed to minimize unwanted reflections.

Let's write \( v^{n+1}(k, j, 0) \) on the artificial boundary, e.g., \( x = 0 \) as is shown in Figure 1, as a linear combination of fields at previous time steps and at \( x \geq 0 \) as:

\[
v^{n+1}(k, j, 0) = a_{01}v^{n+1}(k, j, 1) + a_{02}v^{n+1}(k, j, 2) + a_{10}v^n(k, j, 0) + a_{11}v^n(k, j, 1) + a_{12}v^n(k, j, 2) + a_{20}v^{n-1}(k, j, 0) + a_{21}v^{n-1}(k, j, 1) + a_{22}v^{n-1}(k, j, 2) \tag{1}
\]

where the coefficients \( \{a_{ij}\} (a_{00} = 0) \) are chosen such that reflection from the artificial boundary at \( x = 0 \) is as small as possible. In acoustic cases, eq. (1) is directly applied to the pressure field on the artificial boundary; when being used to absorb elastic energy, eq. (1) is applied to the individual component of an elastic wave. In this scheme, only grid points perpendicular to the boundary are used in the extrapolation process. Attention is also restricted to cases where the extrapolation operator is two steps deep in both time and space, i.e., a \((2,2)\) scheme where the first number refers to the steps in time and the second in space. A more general formulation will be given at the end of this paper. The \((2,2)\) schemes are often used in the literature (Reynolds, 1978; Higdon, 1990; Clayton and Engquist, 1977) because it is very efficient in both computation and memory, and is also easy to code.

Plane wave reflection coefficients

Let's assume the elastic potentials of an incident plane wave in the \((x, z)\) plane to be

\[
Φ = Φ_0 \exp(iωt + ik_α \cos θx + ik_α \sin θz) + R_p \exp(iωt - ik_α \cos θx + ik_α \sin θz) \tag{2}
\]

\[
Ψ = Ψ_0 \exp(iωt + ik_β \cos φx + ik_β \sin φz) + R_s \exp(iωt - ik_β \cos φx + ik_β \sin φz) \tag{3}
\]
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for a P-SV problem. Here $\Phi$ is a dilatation potential and $\Psi$ is the $y$-component of a rotational potential. $\omega$ denotes wave frequency, $k_\alpha = \omega / \alpha$ and $k_\beta = \omega / \beta$ are the compressional and shear wavenumbers, respectively. $\theta$ and $\phi$ are the angles of incidence of the P and S waves, respectively, and are related by

$$\frac{\sin \theta}{\alpha} = \frac{\sin \phi}{\beta}$$

the Snell’s law. $R_p$ and $R_s$ are the P wave and S wave reflection coefficients, respectively.

The displacements in the $x$ and $z$ directions are related to these potentials by the following expressions (Ewing et al., 1957)

$$u = \frac{\partial \Phi}{\partial x} - \frac{\partial \Psi}{\partial z}$$

$$w = \frac{\partial \Phi}{\partial z} + \frac{\partial \Psi}{\partial x}$$

where $u$ is the horizontal displacement and $w$ the vertical.

Let $z = e^{i\omega \Delta t}$ be a one-step shift in time, $z_a = e^{ik_\alpha \cos \theta \Delta x}$ be a one-step shift in space with an apparent compressional velocity, and let $z_b = e^{ik_\beta \cos \phi \Delta x}$ be a one-step shift in space with an apparent shear velocity. By expressing the displacements on the finite difference grid in terms of $z, z_a$ and $z_b$, and substituting them into the boundary condition eq. (1), we obtain the elastic reflection coefficients as

$$R_{pp} = \frac{\xi - \eta}{\xi + \eta} \frac{\Omega_0 + \Omega_1 z_a + \Omega_2 z_a^2}{\Omega_0 + \Omega_1 z_a^{-1} + \Omega_2 z_a^{-2}}$$

$$R_{ps} = \frac{2\xi \eta}{\xi + \eta} \frac{\Omega_0 + \Omega_1 z_b + \Omega_2 z_b^2}{\Omega_0 + \Omega_1 z_b^{-1} + \Omega_2 z_b^{-2}}$$

$$R_{sp} = -\frac{2}{\xi + \eta} \frac{\Omega_0 + \Omega_1 z_b + \Omega_2 z_b^2}{\Omega_0 + \Omega_1 z_a^{-1} + \Omega_2 z_a^{-2}}$$

$$R_{ss} = \frac{\xi - \eta}{\xi + \eta} \frac{\Omega_0 + \Omega_1 z_a + \Omega_2 z_a^2}{\Omega_0 + \Omega_1 z_b^{-1} + \Omega_2 z_b^{-2}}$$

where $R_{pp}$ and $R_{ps}$ are the P to P and P to S reflection coefficients and $R_{sp}$ and $R_{ss}$ are the S to P and S to S reflection coefficients, respectively, and where

$$\Omega_0 = a_{00} z + a_{10} + a_{20} z^{-1} - z$$

$$\Omega_1 = a_{01} z + a_{11} + a_{21} z^{-1}$$

$$\Omega_2 = a_{02} z + a_{12} + a_{22} z^{-1}$$

are the $z$-transforms along columns of the coefficient matrix $\{a_{ij}\}$, and $\xi = \frac{\beta}{\alpha} \cos \theta / \sin \phi$, $\eta = \frac{\beta}{\alpha} \sin \theta / \cos \phi$. It is worthwhile to note that eqs. (4)–(7) agree with Higdon (1990) in the continuous limit $\Delta t \to 0, \Delta x \to 0$ and $\Delta t / \Delta x$ finite.
The reflection coefficients on a finite difference grid have neat structures: (1) the numerator is a space $z$-transform associated with the incident wave; (2) the denominator is another space $z$-transform associated with the reflected wave; (3) the coefficients $I_0$, $\Omega_1$ and $\Omega_2$ are $z$-transforms with respect to time; (4) the numerator represents a wave propagating toward an artificial boundary, therefore it is a polynomial of positive power of $z$; (5) the denominator represents a wave reflected backward into the finite difference domain and is a polynomial of negative power of $z$.

**Transfer Functions Analogy**

Using electrical engineering terminology, the reflection coefficients in eqs. (4)-(7), e.g., $R_{pp}$, can be regarded as the combined transfer functions of two cascaded subsystems shown in the block diagram of Figure 2. The input $x(n)$ is passed to the inverse of a delayed feed-backward subsystem, then in turn, the intermediate result $w(n)$ is fed into an advanced feed-forward subsystem to generate the system output $y(n)$. These two cascaded subsystems can be represented by a pair of difference equations (Oppenheim and Schafer, 1989):

\[
\Omega_0 w(n) + \Omega_1 w(n-1) + \Omega_2 w(n-2) = x(n) \tag{11}
\]

\[
\Omega_0 w(n) + \Omega_1 w(n+1) + \Omega_2 w(n+2) = y(n) \tag{12}
\]

with the first a causal system and the second an anticausal system.

The transfer functions of these two difference equations, obtained by $z_a$-transforming both sides of the above difference equations, are

\[
D_+(z_a) = \frac{1}{\Omega_0 + \Omega_1 z_a^{-1} + \Omega_2 z_a^{-2}} \tag{13}
\]

\[
D_-(z_a) = \frac{1}{\Omega_0 + \Omega_1 z_a + \Omega_2 z_a^2} \tag{14}
\]

respectively. Then by eliminating the $z_a$-transform of $w(n)$, the transfer function of the entire system is

\[
H(z_a) = \frac{D_+(z_a)}{D_-(z_a)}
\]

By inspection, we find that $R_{pp}$, the P to P reflection coefficient, is related to $H(z_a)$ by

\[
R_{pp} = \frac{\xi - \eta}{\xi + \eta} H(z_a) \tag{15}
\]

and similar relationships exist for the other reflection coefficients.

It is worthwhile to note that: (1) for the first subsystem to be stable, the poles of $D_-(z_a)$ must be inside the unit circle $|z_a| = 1$ in a complex $z_a$ plane (Oppenheim and
Schafer, 1989; Robinson and Treitel, 1980); (2) for the same reason, the pole of $D_+(z_a)$ must be outside the unit circle. We can draw the following conclusions for the derived reflection coefficients in eqs. (4)-(7):

- the poles of the reflection coefficients must be on or inside the unit circle,
- the zeros of the reflection coefficients must be on or outside the unit circle,

where we have included the unit circle as a permissible position for both the zeros and poles because, as will be shown later, $z_a$ is defined only on a small segment of the unit circle for an incidence angle from $0^\circ$ up to $90^\circ$.

**DESIGN OF OPTIMAL ABSORBING BOUNDARY CONDITIONS**

**Summation Identity:** The first identity we present is

$$\sum_{i=0,j=0} a_{ij} = 1 \quad (16)$$

i.e., summation of the coefficients on the right hand side of eq. (1) must be an identity.

There are many ways to prove eq. (16). Let's take the limit of $\Delta t \to 0$ and $\Delta x \to 0$, the wave field around the boundary should be the same in the tiny region $(x = 0, x + 2\Delta x)$ and $(t - \Delta t, t + \Delta t)$, which yields eq. (16) from eq. (1). Also imagine that $\Delta t \to 0$ and $\Delta x \to 0$, i.e., $(z, z_a, z_b) \to (1, 1, 1)$, we have the reflection coefficients, e.g., $R_{pp}$,

$$R_{pp} \to \frac{\xi - \eta}{\xi + \eta}$$

for $\Omega_0 + \Omega_1 + \Omega_2 \neq 0$. $R_{pp}$ will be finite at almost all incidence angles if this is true. This case fails to achieve our objective to find appropriate coefficients that minimize the reflection coefficients. For that, we must have $\Omega_0 + \Omega_1 + \Omega_2 = 0$ when $\Delta t \to 0$ and $\Delta x \to 0$, which also yields eq. (16).

**Differentiation Identities:** The second and third identities we present are

$$\sum_{j=0} (a_{0j} - a_{2j}) = 1 \quad (17)$$

and

$$\sum_{i=0} (a_{i0} - a_{i2}) = 1 \quad (18)$$
where eq. (17) is true if no $\partial/\partial t$ term exists in the equivalent differential form of eq. (1), and eq. (18) is true also if no $\partial/\partial x$ term shows up (Cheng, personal communication).

Eqs. (17) and (18) also imply, at angles of incidence that $R_{pp}$ should be zero if $\Delta t = 0$ and $\Delta x = 0$, that

$$R_{pp} \approx O((\Delta t)^2, (\Delta x)^2)$$

as $\Delta t \to 0$ and $\Delta x \to 0$, i.e., the rate of convergence should be at least $O((\Delta t)^2, (\Delta x)^2)$. Simple Taylor expansion of the numerator and denominator of the reflection coefficient in terms of $\Delta t$ and $\Delta x$ is enough to obtain eqs. (17) and (18).

**Minimum Energy Wavelet:** As we will show later, there is a degree of freedom in the choice of coefficients in eq. (1) for a given optimal absorbing ability besides the above three constraints. Whenever this happens, we will impose the energy minimization constraint to the coefficients $(a_{ij})$ as,

$$\sum_{i=0,j=0} a_{ij}^2 = \text{minimum} \quad (19)$$

$\Delta t \to 0$ paradox: Suppose $\Delta t \to 0$ and $\Delta x$ finite. Then,

$$I(\Omega_0) \to 0$$

$$I(\Omega_1) \to 0$$

$$I(\Omega_2) \to 0$$

where $I(.)$ denotes the imaginary part of a quantity in the bracket.

Under these conditions, it can be shown that

$$\left\| \frac{\Omega_0 + \Omega_1 z_a + \Omega_2 z_a^2}{\Omega_0 + \Omega_1 z_a^{-1} + \Omega_2 z_a^{-2}} \right\| \equiv 1$$

for all $z_a$ on the unit circle, i.e., the reflection coefficient (in the acoustic case; in the elastic case there is a factor of $(\xi - \eta)/(\xi + \eta)$ difference) will be unity in magnitude no matter what $\Delta x$ may be. This observation has two implications: (1) keeping $\Delta t$ very small alone will reduce the effectiveness of an absorbing boundary although interior time integration will be more accurate; (2) the optimal absorbing condition exists only where $\alpha \Delta t/\Delta x$ is finite. Higdon (1986) observed a similar phenomenon by taking $\omega \to 0$. In his analysis, he concluded that a substantial reflection occurs at low frequencies.
Recall that
\[ z_a = e^{ik_a \cos \theta \Delta x} \]
where \( \theta \) is the angle of incidence of a plane wave impinging on a boundary.

As \( \theta \) varies from 0° to 90°, in the complex plane, \( z_a \) lies between \((\cos(k_a \Delta x), \sin(k_a \Delta x))\) and (1,0) along the unit circle. In terms of the phase angle \( \theta \) (with the real axis), \( z_a \) lies on the unit circle with
\[ 0 \leq \theta_a \leq k_a \Delta x. \]

\( z_b \), the one-step shift with the apparent shear velocity, lies in
\[ 0 \leq \theta_b \leq k \beta \Delta x \]

and \( \theta_a < \theta_b \) because \( \alpha > \beta \).

The reflection coefficients, e.g., \( R_{pp} \), have two non-zero zeros and two poles in the complex \( Z \) plane. They are at
\[ z_c^\pm = \frac{\Omega_1 \pm \sqrt{\Omega_1^2 - 4 \Omega_0 \Omega_2}}{2 \Omega_2} \]
for the zeros, and
\[ z_p^\pm = \frac{\Omega_1 \pm \sqrt{\Omega_1^2 - 4 \Omega_0 \Omega_2}}{2 \Omega_0} \]
for the poles. Note that the difference between the zeros and poles is just a factor of \( \Omega_0 / \Omega_2 \).

The location of the zeros and poles completely determines the reflection coefficients. For example, the magnitude of the reflection coefficient \( R_{pp} \) is proportional to the ratio of
\[ \frac{|z_a - z_c^+| |z_a - z_c^-|}{|z_a - z_p^+| |z_a - z_p^-|} \]
where the terms between the vertical bars are distances between \( z_a \) and the zeros and the poles as is shown in Figure 3.

Requirements for the locations of zeros and poles are: (1) the zeros are on or outside the unit circle; (2) the poles are on or inside the unit circle; (3) for an optimal boundary condition, both the zeros are on the segment of the unit circle where \( z_a \) is defined such that there is a maximal cancellation of the reflection coefficients in the numerator. This is analogous to that in Higdon (1986). Since the poles are dependent on the zeros, their locations inside or on the unit circle are not arbitrary. Optimal locations of the zeros and poles do exist at which the reflection coefficients are (local) minima.
Conjugate Gradient Optimization

Optimal $\Omega_0, \Omega_1$ and $\Omega_2$ are chosen such that

$$
\sum_{\theta_i=0}^{85^\circ} w(\theta_i) \left[ \frac{\Omega_0 + \Omega_1 z_a + \Omega_2 z_a^2}{\Omega_0 + \Omega_1 z_a^{-1} + \Omega_2 z_a^{-2}} - \frac{\bar{\Omega}_0 + \bar{\Omega}_1 z_a^{-1} + \bar{\Omega}_2 z_a^{-2}}{\bar{\Omega}_0 + \bar{\Omega}_1 z_a + \bar{\Omega}_2 z_a^2} \right]^m = \Gamma = \text{minimum} \quad (22)
$$

subject to the constraints discussed in the above sections. Where $m \geq 1$ is an integer, $w(\theta_i)$ is a positive weighting function. The minimizer is a summation, up to $85^\circ$ incidence angle, of the magnitude of the reflection coefficient in the acoustic case. We can minimize any or a combination of the four reflection coefficients in the elastic case, the choice then would be problem dependent.

Given that the function in eq. (22) and its partial derivatives are easily computed, the conjugate gradient method is an appropriate choice to minimize $\Gamma$ numerically. We modified the code published in Numerical Recipes (Press et al., 1989) slightly, so as to accommodate the constraints such that the zeros are near to the domain of $z_a$ for $0 \leq \theta_i \leq 85^\circ$. The initial values for $\Omega_0$, $\Omega_1$ and $\Omega_2$ are nearly zero. The choice of the weighting function $w(\theta)$ is $e^{-10(1-\cos^2 \theta)}$ and $m$, the power raised in eq. (22), is 2.

For a practical problem with $\alpha = 3000$ m/s, $\beta = 2000$ m/s, $\Delta t = 0.0005$ s, $\Delta z = 10$ m and $\omega = 2\pi \times 20$ Hz, we find

$$
\Omega_0 = (-0.008179450, -0.018289154),
\Omega_1 = (+0.028303795, +0.028303849),
\Omega_2 = (-0.018289177, -0.008179528)
$$

at which the $\Gamma$ is a local or global minimum.

Results Analysis

Zeros and poles diagram: Given the $\Omega_i$, we can compute the location of zeros and poles for this optimal absorbing condition. We plot these zeros and poles in a complex $z$-plane (Figure 4a). As a comparison, we also compute the zeros and poles of Reynolds' (Figure 4b) and Higdon's (Figure 4c) absorbing conditions by using equation (18c) in Reynolds (1978) and equation (12) with $\beta_1 = 1, \beta_2 = \alpha/\beta = 1.5$ in Higdon (1991), respectively. We find that for the optimal absorbing boundary condition obtained by the conjugate gradient minimization, the two zeros are located exactly on the segment of the unit circle where $z_a$ is defined for an angle of incidence between $0^\circ$ and $90^\circ$. Reynolds' and Higdon's absorbing boundary conditions don't have this property. There is only one zero on the unit circle slightly above the real axis for Reynolds' boundary
condition, while for Hidgon's absorbing condition two zeros remain outside the unit circle. The two poles of the optimal absorbing condition are also located on the unit circle at the conjugated positions of the two zeros. For Reynolds' boundary condition, one pole is almost on the unit circle and slightly below the real axis, very close to the domains of \( z_a \) and \( z_b \). This explains why Reynolds' boundary condition behaves poorly as \( \Delta t \to 0 \), because this particular pole comes increasingly closer to the real axis.

**Acoustic Reflection Coefficients:** Figure 5 plots the reflection coefficients of the optimal, Reynolds', and Higdon's absorbing boundary conditions in the acoustic case. The horizontal axis in this plot is the angle of incidence, the vertical axis is \( 20 \log_{10}(|R_{pp}| + \epsilon) \) where \( \epsilon = 10^{-20} \) is a small positive number to avoid the singularity of the log function. The reflection coefficient of the optimal absorbing boundary condition has two zeros and is generally 10-20 dB less in magnitude than Higdon's absorbing boundary condition, which in turn has a better performance by about 10 dB (less) over Reynolds' boundary condition. An exception occurs at an angle near grazing incidence where Reynolds' absorbing boundary condition has a smaller reflection. Comparing the plots in the papers by Reynolds (1978) and Higdon (1991), we find that the reflection coefficients on a discrete finite difference grid are different from those derived from an analytical boundary condition. For example, in the continuous case the acoustic reflection coefficient in both Reynolds' and Higdon's absorbing boundary conditions has a zero at normal incidence \( \theta = 0^\circ \), while on a discrete finite difference lattice this is no longer the case.

**Elastic Reflection Coefficients:** When used to absorb elastic energies, the absorbing condition in eq. (1) is applied to each elastic wave component. Figure 6a shows the \( P \to P \) reflection coefficients for the three absorbing boundary conditions as discussed in previous examples. We find that besides the two zeros at \( z_a = z_a^\pm \), there is a physical zero in \( R_{pp} \) at which \( \xi = \eta \), i.e., there is no reflection in the P wave. Still the optimal absorbing boundary condition outperforms other boundary conditions by approximately 10-20 dB less in magnitude of the reflection coefficients.

Figure 6b shows the \( P \to S \) reflection coefficients for the optimal, Reynolds' and Higdon's absorbing boundary conditions. \( R_{ps} \) is generally small for all three boundary conditions, although the optimal is again better than Higdon's and Reynolds'.

In Figure 7a and 7b, we plot the \( S \to P \) and \( S \to S \) reflection coefficients, respectively, for the three absorbing boundary conditions. For the particular choice of parameters in this paper, Reynolds' boundary condition behaves very poorly for \( |R_{sp}| > 1 \) at an incidence angle \( \phi \sim \sin^{-1} \beta/\alpha \). Analysis shows that the smaller the time step \( \Delta t \) and \( \beta/\alpha \), the more unstable the Reynolds absorbing boundary condition, as has been reported by Mahrer (1986). Obviously for a general purpose finite difference modeling
code, Reynolds' absorbing boundary condition is not a good choice to absorb artificial reflections (the instability of Clayton and Engquist (1977) absorbing boundary condition was also reported in Mahrer (1986) and Emerman and Stephen (1983) ). There is a physical zero in \( R_{ss} \) corresponding to the case where no S wave reflection exists. The optimal absorbing boundary condition has two additional zeros in \( R_{ss} \) at angles of incidence corresponding to \( \theta_0 = \pm \theta^\pm \). At small incidence angles, Higdon's boundary condition has smaller \( R_{sp} \) and \( R_{ss} \) reflection coefficients because it is designed to absorb a normal incident S wave. At large angles of incidence, the optimal is better. This doesn't mean that the Higdon (1991) absorbing boundary condition is better at absorbing normal incident S waves, because the optimal absorbing boundary condition in this particular example is designed for a maximum absorption of the incident P wave. By properly locating the zeros on the unit circle, we can have better S wave absorption ability with some sacrifice of the P wave absorption. With the fast algorithm given in the next section, we can compute the coefficients \( \{a_{ij}\} \) for any given locations of the zeros on the unit circle.

**DISCUSSION**

**Relationships between zeros and poles**

Suppose the two zeros of the reflection coefficient \( R_{pp} \), \( z^\pm \), are given, the two poles are determined by

\[
z^\pm_p = \frac{1}{z^\pm_c}
\]

i.e., the zeros are paired with the poles in such a way that one is the inverse of the other. The proof is straightforward by making use of \( \Omega_1/\Omega_2 = -(z^+_c + z^-_c) \) and \( \Omega_0/\Omega_2 = z^+_c z^-_c \).

The implications of relationship eq. (23) are: (1) if the zeros are outside the unit circle, the poles must be inside the unit circle; (2) the magnitude of a pole of \( R_{pp} \) is the inverse of that of a zero, and the phase of a pole is the negative of that of a zero; (3) if the zeros are on the unit circle, so are the poles. More importantly, in the last case, the phase angles of the zeros determine the properties of the reflection coefficients.

The poles and zeros plots in Figure 4 clearly show these properties.

**Properties of an optimal absorbing boundary condition**

We will proceed in this paragraph by claiming that *for an absorbing boundary condition to be optimal, the zeros of the reflection coefficients must be on the unit circle, and if \( k_A \Delta x < \frac{\pi}{2} \), the zeros also must be in the first quadrant.* Here \( k_A \Delta x < \frac{\pi}{2} \) comes from the
requirement that at least 5 points per wavelength are needed to reduce grid dispersion for the commonly used 4th order differentiation scheme (Virieux, 1986; Levander, 1988).

To prove this statement, it is advantageous to rewrite the reflection coefficient (acoustic case) as

\[
R_{pp} = \frac{(z_a - z^+)(z_a - z^-)}{(z_a^{-1} - z^+)(z_a^{-1} - z^-)}
\]  

where eq. (23) has been used in the derivation. As a reminder, the domain of \(z_a\) is on a segment of the unit circle with a phase angle between \((0, k_\alpha \Delta x]\).

Let \(z^+_a = r_+e^{i\theta_+}, z^-_a = r_-e^{i\theta_-}\), the statement says that for fixed \(\theta_+\) and \(\theta_-\) in \((0, k_\alpha \Delta x]\), the minimum magnitude of eq. (24) occurs at \(r_+ = r_- = 1\). Analytical proof is straightforward and mathematically involved. We will adopt a graphic proof shown in Figure 8. In this figure the open circle represents one of the two zeros of the reflection coefficient in eq. (24), and the two solid circles represent \(z_a\) and \(z_a^{-1}\), respectively. As the zero of eq. (24) moves toward infinity in the first quadrant, the ratio of \(|z_a - z^+_a| / |z_a^{-1} - z^+_a|\) increases monotonically to 1. A minimum exists only at \(|z^+_a| = 1\).

A fast algorithm

To render our method practically useful, a technique other than the conjugate gradient optimization is necessary. Advantages can be gained by making use of the properties of an optimal absorbing boundary condition. We propose the following algorithm to design a useful optimal boundary condition to absorb artificial reflections. The inputs to the algorithm are two physical incidence angles \(\theta_+\) and \(\theta_-\) at which either \(R_{pp}\) or \(R_{ss}\) (depending on the user's choice) is zero, in addition to the dimensionless time step \(\Delta t = \omega \Delta t\) and grid size \(\Delta x = \nu / \alpha \Delta x\) for maximum P wave absorptions, or \(\Delta x = \nu / \beta \Delta x\) for maximum S wave absorptions. The phase angles \(\theta_+\) and \(\theta_-\) of the two zeros are related to the physical incidence angles \(\theta^\pm\) by

\[
\theta^\pm = \Delta x \cos \theta^\pm
\]

It is easy to show that

\[
\frac{a_{00}z + a_{10} + a_{20}z^{-1} - z}{a_{02}z + a_{12} + a_{22}z^{-1}} = \cos(\theta_+ + \theta_-) + i \sin(\theta_+ + \theta_-)
\]

and

\[
\frac{a_{01}z + a_{11} + a_{21}z^{-1}}{a_{02}z + a_{12} + a_{22}z^{-1}} = -(\cos \theta_+ + \cos \theta_-) - i(\sin \theta_+ + \sin \theta_-)
\]

where eqs. (8)-(10) are used, and \(z = e^{i\Delta t}\).
The above two equations offer 4 constraints on the coefficients \( \{a_{ij}\} \) where 8 are unknown \( (a_{00} = 0) \). The other 4 constraints come from the three identities in eq. (16), eq. (17) and eq. (18), and one from the minimum energy criterion in eq. (19). The algorithm to compute \( \{a_{ij}\} \) is presented in Appendix A. The absorbing boundary condition designed with this algorithm is guaranteed to be optimal in the sense that the artificial reflections are at least local minimums. The actual global minimum in eq. (22) is dependent on the weighting function and the power raised. Table 1 lists the \( \{a_{ij}\} \) for the optimal absorbing boundary condition shown in Figure 4a.

**Generalization to \((m, m)\) schemes**

So far, we are focusing our attention on the \((2, 2)\) scheme, i.e., the extrapolation on the artificial boundary has two steps "deep" in both time and space. Generalization to a scheme that has \( m \) steps "deep" in both time and space can be derived and the results are:

\[
R_{pp} = \frac{\xi - \eta}{\xi + \eta} \frac{\sum_{j=0}^{m} \Omega_j z_a^j}{\sum_{j=0}^{m} \Omega_j z_a^{-j}}
\]

\[
R_{ps} = -\frac{2\xi \eta}{\xi + \eta} \frac{\sum_{j=0}^{m} \Omega_j z_a^j}{\sum_{j=0}^{m} \Omega_j z_b^{-j}}
\]

\[
R_{sp} = \frac{\xi}{\xi + \eta} \frac{\sum_{j=0}^{m} \Omega_j z_b^j}{\sum_{j=0}^{m} \Omega_j z_a^{-j}}
\]

\[
R_{ss} = \frac{\xi - \eta}{\xi + \eta} \frac{\sum_{j=0}^{m} \Omega_j z_b^j}{\sum_{j=0}^{m} \Omega_j z_b^{-j}}
\]

where

\[
\Omega_j = \sum_{i=0}^{m} a_{ij} z^{1-i} - \delta_{j0} z
\]

Here \( \delta_{j0} = \begin{cases} 1 & j = 0 \\ 0 & \text{otherwise} \end{cases} \) is the Kronecker's delta. The properties of the \((m, m)\) scheme are similar to those of the \((2, 2)\) scheme discussed previously. For example, for a \((m, m)\) scheme to be optimal, the \( m \) zeros of the reflection coefficients must be on the segment of the unit circle with phase angles between \( (0, k\alpha \Delta z) \), and the poles are at the conjugated positions of the zeros.

**AN EXAMPLE**

In this section, we will give an example of 3D elastic finite difference modeling on an nCUBE parallel computer. The objective is to compare the optimal, Higdon's,
Peng and Toksöz

and Reynolds’ absorbing boundary conditions with a realistic simulation. We used the stress-velocity formulation of Virieux (1986) and Levander (1988) on a staggered grid. The scheme has a fourth-order accuracy in space and second-order accuracy in time. Dispersion analysis suggests that the shortest wavelengths in the model be sampled at 5 grid points per wavelength. The boundary conditions on the six surfaces of a 3D volume can be either symmetric, stress free, or absorbing. The source can be either a direct force or an explosion or any combination of both. The code is optimized to minimize internode communications and I/O on a parallel computer. For a 3D elastic modeling with 100 × 100 × 100 grids and 2000 time steps, it takes about 42 minutes on a 64 node nCUBE-2 at the Geophysical Center for Parallel Processing, Earth Resources Laboratory, Massachusetts Institute of Technology.

In this example, we simulate the elastic wave propagation in an unbounded homogeneous medium with compressional velocity \( c = 3000 \) m/s, shear velocity \( \beta = 2000 \) m/s, and density \( \rho = 2000 \) kg/m\(^3\). We use an explosive source. The source function is a delayed Ricker wavelet \( s(t) = (2\pi f_0^2(t - t_0)^2 - 1)e^{-\pi^2 f_0^2(t-t_0)^2} \) with central frequency \( f_0 = 20 \) Hz and time delay \( t_0 = f_0^{-1} \). The size of the 3D volume is 960 m in each dimension. The time step chosen is \( \Delta t = 0.0005 \) s and grid size \( \Delta x = 10 \) m. The source is at coordinate \((x_s, y_s, z_s) = (240 \text{ m, 240 m, 240 m})\). All the six surfaces are absorbing boundaries with either the optimal, Reynolds’, or Higdon’s boundary condition.

Shown in Figure 9, 10 and 11 are snapshots taken at propagational time 0.15, 0.20, 0.25 and 0.30 s respectively. The snapshots are the vertical particle velocities in the x-z plane at \( y = 240 \) m, and are blown up by a factor of ten to make reflections from the artificial boundaries visible. In these plots only the first arrival is physical, all the others are artificial reflections from boundaries. In the simulation with the Reynolds’ absorbing boundary condition, artificial reflection is about one tenth of the incident wave and is clearly visible in the amplified snapshots (Figure 9). The artificial reflection is much smaller in the simulation with Higdon’s absorbing boundary condition, which is about one thirtieth of the incident wave (Figure 10). The simulation with the optimal absorbing boundary condition, as shown in Figure 11, has a smaller artificial reflection than both the Higdon and Reynolds absorbing boundary conditions.

CONCLUSIONS

A method is presented in this paper to design optimal absorbing boundary conditions to model acoustic and elastic wave propagation in 2D and 3D media using the finite difference method. At a given time step, the field on an artificial boundary is expressed as a linear combination of the field at previous time steps and interior grid points. The reflection coefficients are found to be identical with the transfer functions of two cascaded systems: one is the inverse of a causal and delayed feed-backward system, the other is an anticausal and advanced feed-forward system. The reflection from an artificial
Optimal Absorbing Boundary

boundary is determined by the locations of the zeros and the poles of the reflection coefficients in a complex \( z \) plane. It is found that for an absorbing boundary condition to be optimal the zeros of the reflection coefficients must be on the segment of the unit circle with phase angles between \( (0, k \Delta x) \). A fast algorithm is given to compute the unknown coefficients in the boundary extrapolation scheme. Comparisons between the optimal absorbing boundary condition and the Reynolds' and Higdon's absorbing boundary conditions are given, both with evaluations of the reflection coefficients and with a realistic simulation of elastic wave propagation in a 3D medium.

The optimal absorbing boundary condition we design yields about 10 dB smaller in magnitude of reflection coefficients than the Higdon's absorbing boundary condition and about 20 dB smaller than the Reynolds' absorbing boundary condition. The simulations of 3D elastic wave propagation using finite difference show that the optimal absorbing boundary condition has a smaller artificial reflection than the Reynolds and Higdon absorbing boundary conditions.

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APPENDIX A

Determination of \{a_{ij}\}

In this appendix, we present a method to determine \{a_{ij}\}. The problem is a quadratic minimization subject to linear constraints. In this method, equation eq. (19) in the text is replaced by a linear equation

$$\sum_{i=0, j=0}^{\infty} (-1)^{i+j} a_{ij} = \lambda$$

(A - 1)

where \(\lambda\) is to be determined. Any linear function will serve the purpose as long as it is independent of the other 7 equations.

In terms of \(\lambda\), \{a_{ij}\} can be solved by

$$\begin{bmatrix}
  a_{01} \\
  a_{02} \\
  a_{10} \\
  a_{11} \\
  a_{12} \\
  a_{20} \\
  a_{21} \\
  a_{22}
\end{bmatrix} = \begin{bmatrix}
  1 \\
  1 \\
  1 \\
  1 \\
  \lambda \\
  R_z \\
  I_z \\
  0
\end{bmatrix}$$

where

$$A = \begin{bmatrix}
  1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
  1 & 1 & 0 & 0 & 0 & -1 & -1 & -1 \\
  0 & -1 & 1 & 0 & -1 & 1 & 0 & -1 \\
  -1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 \\
  0 & -(R_x R_z - I_x I_z) & 1 & 0 & -R_x & R_z & 0 & -(R_x R_z + I_x I_z) \\
  0 & -(R_x I_z + R_z I_x) & 0 & 0 & -I_z & -I_z & 0 & -(R_z I_z - R_z I_z) \\
  R_z & -(R_y R_z - I_y I_z) & 0 & 1 & -R_y & 0 & R_z & -(R_y R_z + I_y I_z) \\
  I_z & -(R_y I_z + R_z I_y) & 0 & 0 & -I_y & 0 & -I_z & -(R_z I_y - R_y I_z)
\end{bmatrix}$$

and \(R_x = \cos \Delta t, I_z = \sin \Delta t, R_x = \cos(\vartheta_+ + \vartheta_-), I_x = \sin(\vartheta_+ + \vartheta_-), R_y = -\cos \vartheta_+ + \cos \vartheta_-\), and \(I_y = -\sin \vartheta_+ + \sin \vartheta_-\).

The solution of the above 8 x 8 matrix equation can be expressed as

$$a_{ij} = \gamma_{ij}^{(0)} + \gamma_{ij}^{(1)} \lambda$$

where \(\gamma_{ij}^{(0)}\) and \(\gamma_{ij}^{(1)}\) are derived from the inverse of \(A\).
Optimal Absorbing Boundary

The choice of $\lambda$ is to make eq. (19) minimum, which yields

$$\lambda = \frac{\sum_{i=0,j=0}^{\text{max}} \gamma_{ij}^{(0)} \gamma_{ij}^{(1)}}{\sum_{i=0,j=0}^{\text{max}} \gamma_{ij}^{(1)} \gamma_{ij}^{(1)}}$$

Thus the optimal coefficients are computed by

$$a_{ij} = \gamma_{ij}^{(0)} \frac{\sum_{k=0,l=0}^{\text{max}} \gamma_{kl}^{(0)} \gamma_{ij}^{(1)}}{\sum_{k=0,l=0}^{\text{max}} \gamma_{kl}^{(1)} \gamma_{kl}^{(1)}}.$$  \hspace{1cm} (A-2)

<table>
<thead>
<tr>
<th>$a_{ij}$</th>
<th>$j=0$</th>
<th>$j=1$</th>
<th>$j=2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i=0$</td>
<td>0.0000000000</td>
<td>-0.0893569160</td>
<td>-0.6916645269</td>
</tr>
<tr>
<td>$i=1$</td>
<td>1.6376375943</td>
<td>0.2867676972</td>
<td>1.6376375943</td>
</tr>
<tr>
<td>$i=2$</td>
<td>-0.6916645269</td>
<td>-0.0893569160</td>
<td>-1.0000000000</td>
</tr>
</tbody>
</table>

Table 1: List of coefficients for the optimal absorbing boundary condition whose zero-pole plot is identical with Figure 4a. Physical parameters are: $\alpha = 3000$ m/s, $\beta = 2000$ m/s, $\omega = 2\pi \times 20$ Hz, $\Delta t = 0.0005$ s and $\Delta x = 10$ m.
Figure 1: A stencil for updating a boundary grid at $x = 0$ for a finite difference modeling of wave equation. The unknown data (solid circle) is computed by the 8 known values (open circle) according to equation eq. (1) in the text.
Figure 2: The reflection coefficient, e.g., $R_{pp}$, is identical with the transfer function of two cascaded systems. The first is the inverse of a causal feed-backward system with delay. The second is an anticausal feed-forward system with advance.
Figure 3: Geometrical representations in a complex z plane of the elastic reflection coefficients from an artificial boundary.
Figure 4: Zeros and poles in a complex $z$ plane of the optimal, Reynolds', and Higdon's absorbing boundary conditions.
Acoustic Case (P to P Reflection Coefficients)

Figure 5: Acoustic reflection coefficients as a function of incidence angle for the optimal, Reynolds', and Higdon's absorbing boundary conditions. The solid line is the optimal, the long dashed line the Reynolds' and the short dashed line the Higdon's. The vertical axis is magnitudes in dB of the reflection coefficients.
Figure 6: Elastic reflection coefficients $R_{pp}$ and $R_{ps}$ as a function of incidence angle for the optimal, Reynolds', and Higdon's absorbing boundary conditions.
Figure 7: Elastic reflection coefficients $R_{sp}$ and $R_{ss}$ as a function of incidence angle for the optimal, Reynolds', and Higdon's absorbing boundary conditions.
Figure 8: A graphic proof of the statement that the zeros of an optimal absorbing boundary condition are on the unit circle. It is obvious that $w_1 = |z_a - z_c|$ increases faster than $w_2 = |z_a^{-1} - z_c|$ as $z_c \to \infty$ in the first quadrant.
Figure 9: Snapshots of a 3D elastic finite difference simulation on an nCUBE parallel computer with Reynolds' absorbing boundary condition. Shown in the snapshots are the vertical particle velocities. The snapshots are taken at propagational time 0.15, 0.20, 0.25 and 0.30 s, respectively, and are blown up by a factor of ten.
Figure 10: Same as in Figure 9 but with Higdon's absorbing boundary condition.
Figure 11: Same as in Figure 9 but with the optimal absorbing boundary condition.